OpenCMISS-iron examples and tests used by *OpenCMISS* developers at University of Stuttgart, Germany

Christian Bleiler[*], Dr.-Ing. Nehzat Emamy[†], Andreas Hessenthaler[*], Thomas Klotz[*], Aaron Krämer[‡], Benjamin Maier[†], Sergio Morales[*], Mylena Mordhorst[*], Harry Saini[*]

July 10, 2017
18:10

CONTENTS

1 Introduction 5
1.1 Cmgui files for cmgui-2.9 . . . 5
1.2 Variations to consider . . . 5
1.3 Folder structure . . . 6
2 Progress 7
2.1 Equations to test . . . 7
2.2 Setting up a new test . . . 7
2.3 Long-term goals . . . 8
3 Diffusion equation 9
3.1 Equation in general form . . . 9
3.2 Example-0001 [VALIDATED] . . . 10
3.2.1 Mathematical model - 2D . . . 10
3.2.2 Mathematical model - 3D . . . 10
3.2.3 Computational model . . . 10
3.2.4 Result summary . . . 11
3.3 Example-0001-u [VALIDATED] . . . 14
3.3.1 Mathematical model - 2D . . . 14
3.3.2 Mathematical model - 3D . . . 14
3.3.3 Computational model . . . 14
3.3.4 Result summary . . . 15
3.4 Example-0002 [VALIDATED] . . . 18

[*] Institute of Applied Mechanics (CE), University of Stuttgart, Pfaffenwaldring 7, 70569 Stuttgart, Germany
[†] Institute for Parallel and Distributed Systems, University of Stuttgart, Universitätsstraße 38, 70569 Stuttgart, Germany
[‡] Lehrstuhl Mathematische Methoden für komplexe Simulation der Naturwissenschaft und Technik, University of Stuttgart, Allmandring 5b, 70569 Stuttgart, Germany

3.4.1 Mathematical model - 2D 18
3.4.2 Mathematical model - 3D 18
3.4.3 Computational model 18
3.4.4 Result summary 19
3.5 Example-0003 [COMPILES] 22
3.5.1 Mathematical model - 2D 22
3.5.2 Mathematical model - 3D 22
3.5.3 Computational model 22
3.5.4 Result summary 23
3.6 Example-0004 [VALIDATED] 26
3.6.1 Mathematical model - 2D 26
3.6.2 Computational model 26
3.6.3 Result summary 26
3.7 Example-0005 [VALIDATED] 28
3.7.1 Mathematical model - 2D 28
3.7.2 Mathematical model - 3D 28
3.7.3 Computational model 28
3.7.4 Result summary 29
3.8 Example-0011 [RUNS] 32
3.8.1 Mathematical model - 2D 32
3.8.2 Mathematical model - 3D 32
3.8.3 Computational model 32
3.8.4 Result summary 33
4 Linear elasticity 36
4.1 Equation in general form 36
4.2 Example-0101 [PLAUSIBLE] 37
4.2.1 Mathematical model 37
4.2.2 Computational model 37
4.2.3 Results 38
4.2.4 Validation 38
4.3 Example-0102 [PLAUSIBLE] 41
4.3.1 Mathematical model 41
4.3.2 Computational model 41
4.3.3 Results 42
4.3.4 Validation 43
4.4 Example-0111 [PLAUSIBLE] 45
4.4.1 Mathematical model 45
4.4.2 Computational model 45
4.4.3 Results 46
4.4.4 Validation 47
4.5 Example-0112 [PLAUSIBLE] 49
4.5.1 Mathematical model 49
4.5.2 Computational model 49
4.5.3 Results 50
4.5.4 Validation 51
5 Finite elasticity 53
6 Navier-Stokes flow 54
6.1 Equation in general form 54
6.2 Example-0302-u [COMPILES] 55
6.2.1 Mathematical model - 2D 55
6.2.2 Mathematical model - 3D 55
6.2.3 Computational model 55
6.2.4 Result summary 56

7 Monodomain 57
8 CellML model 58

LIST OF FIGURES

Figure 1 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0]. 11
Figure 2 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0]. 12
Figure 3 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0]. 12
Figure 4 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0]. 13
Figure 5 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0]. 15
Figure 6 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0]. 16
Figure 7 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0]. 16
Figure 8 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0]. 17
Figure 9 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0]. 19
Figure 10 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0]. 20
Figure 11 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0]. 20
Figure 12 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0]. 21
Figure 13 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0]. 23
Figure 14 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0]. 24
Figure 15 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0]. 24
Figure 16 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0]. 25
Figure 17 2D results, iron reference w/ command line arguments [8 4 0 2 0]. 27
Figure 18 2D results, current run w/ command line arguments [8 4 0 2 0]. 27
Figure 19 2D geometry and mesh. 29
Figure 20 2D results, iron reference w/ command line arguments [2 2 0]. 29
Figure 21 2D results, current run w/ command line arguments [2 2 0]. 30
Figure 22 3D geometry (unit cube) and mesh. 30
Figure 23 3D results, iron reference w/ command line arguments [3 2 0]. 31
Figure 24 3D results, current run w/ command line arguments [3 2 0]. 31

Figure 25 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0 1 1]. 34
Figure 26 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0 1 1]. 34
Figure 27 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0 1 1 1]. 35
Figure 28 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0 1 1 1]. 35
Figure 29 Results, iron 2D fine mesh. 38
Figure 30 Results, iron 3D fine mesh. 38
Figure 31 Results, Abaqus 2D fine mesh. 39
Figure 32 Results, abaqus 3D fine mesh. 40
Figure 33 Results, iron 2D fine mesh. 42
Figure 34 Results, iron 3D fine mesh. 42
Figure 35 Results, Abaqus 2D fine mesh. 43
Figure 36 Results, abaqus 3D fine mesh. 44
Figure 37 Results, iron 2D fine mesh. 46
Figure 38 Results, iron 3D fine mesh. 46
Figure 39 Results, Abaqus 2D fine mesh. 47
Figure 40 Results, abaqus 3D fine mesh. 48
Figure 41 Results, iron 2D fine mesh. 50
Figure 42 Results, iron 3D fine mesh. 50
Figure 43 Results, Abaqus 2D fine mesh. 51
Figure 44 Results, abaqus 3D fine mesh. 52

LIST OF TABLES

Table 1 Quantiative error between Abaqus 2017 and iron simulations for linear elastic uniaxial extenions 39
Table 2 Quantiative error between Abaqus 2017 and iron simulations for linear elastic shear 44
Table 3 Quantiative error between Abaqus 2017 and iron simulations for linear elastic uniaxial extenions 48
Table 4 Quantiative error between Abaqus 2017 and iron simulations for linear elastic shear 52

1 INTRODUCTION

This document contains information about examples used for testing *OpenCMISS-iron*. Read: How-to[1] and [1].

1.1 Cmgui files for cmgui-2.9

1.2 Variations to consider

- Geometry and topology
  - 1D, 2D, 3D
  - Length, width, height
  - Number of elements
  - Interpolation order
  - Generated or user meshes
  - quad/hex or tri/tet meshes
- Initial conditions
- Load cases
  - Dirichlet BC
  - Neumann BC
  - Volume force
  - Mix of previous items
- Sources, sinks
- Time dependence
  - Static
  - Quasi-static
  - Dynamic
- Material laws
  - Linear
  - Nonlinear (Mooney-Rivlin, Neo-Hookean, Ogden, etc.)
  - Active (Stress, strain)
- Material parameters, anisotropy
- Solver
  - Direct
  - Iterative
- Test cases
  - Numerical reference data
  - Analytical solution
- A mix of previous items

1 https://bitbucket.org/hessenthaler/opencmiss-howto

1.3 Folder structure

TBD..

2 PROGRESS

People working on setting up tests in alphabetical order (surnames) with initials:

- CB : Christian Bleiler
- NE : Dr.-Ing. Nehzat Emamy
- AH : Andreas Hessenthaler
- TK : Thomas Klotz
- AK : Aaron Krämer
- BM : Benjamin Maier
- SM : Sergio Morales
- MM : Mylena Mordhorst
- HS : Harry Saini

2.1 Equations to test

Test single-physics problems before multi-physics problems!

- Diffusion equation (Laplace, Poisson, Generalized Laplace, ALE Diffusion, etc.)
- Linear elasticity equation (compressible and incompressible)
- Finite elasticity equation (compressible and incompressible Mooney-Rivlin, etc.)
- Navier-Stokes equation (ALE, Stokes, etc.)
- Monodomain equation
- CellML models
- Skeletal muscle models
- Fluid-structure interaction
- etc.

2.2 Setting up a new test

Use the following guideline to set up a new test:

1. Check if it is already there
2. Talk to other developers
3. Create a new subfolder examples/example-oxxx
4. Document the setup (computational domain, etc.) in examples/example-oxxx/doc/example.tex
5. Set up example with all parameters as command line arguments, see Section 1.2

6. Set up reference results (CHeart, Abaqus, analytical solution, etc.)
7. Set up script to run all tests in your example directory
8. Set up script to perform comparison between iron results and reference results
9. Set up visualization scripts
10. Compile, run, test, visualize your example
11. Compile, run, test, visualize all examples

For each example, progress is documented in the respective section titles with the following `TAG`:

- `DOCUMENTED`: finish the documentation of the example (spatial domain, number of time steps, boundary conditions, etc.
- `COMPILES`: example compiles (for default parameters)
- `RUNS`: example runs (for default parameters)
- `CONVERGES`: no convergence issues (for default parameters, results not plausible)
- `PLAUSIBLE`: results look sensible (for default parameters)
- `VALIDATED`: for all parameter sets it gives the correct results as compared to CHeart/Abaqus/analytical solution (includes visualization scripts, run scripts, comparison scripts, documentation!, ...)

Move all tags `CONVERGE, PLAUSIBLE` to `VALIDATED`.

Next steps include:

- Everybody runs everything!
- Meeting with Oliver
- Meeting with Auckland

2.3 Long-term goals

- Different testing targets

  `SMALL` : small, fast tests

  `BIG` : same as before; further, bigger and more complex geometries, convergence analysis

  `PARALLEL` : same as before but in parallel
- Add more examples/those which were on the agenda but not started
- Jenkins continuous testing, integration and deployment

  test `SMALL/BIG/PARALLEL` targets

  integrate with GitHub (pull-requests triggers Jenkins, merge on success)

3 DIFFUSION EQUATION

3.1 Equation in general form

The governing equation is,

$$\partial_t u + \nabla \cdot [\boldsymbol{\sigma} \nabla u] = f, \tag{1}$$

with conductivity tensor $\boldsymbol{\sigma}$. The conductivity tensor is,

- defined in material coordinates (fibre direction),
- diagonal,
- defined per element.

3.2 Example-0001 `[VALIDATED]`

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.2.1 *Mathematical model - 2D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0,2] \times [0,1], \tag{2}$$

with boundary conditions

$$u = 0 \qquad x = y = 0, \tag{3}$$
$$u = 1 \qquad x = 2, y = 1. \tag{4}$$

No material parameters to specify.

3.2.2 *Mathematical model - 3D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0,2] \times [0,1] \times [0,1], \tag{5}$$

with boundary conditions

$$u = 0 \qquad x = y = z = 0, \tag{6}$$
$$u = 1 \qquad x = 2, y = z = 1. \tag{7}$$

No material parameters to specify.

3.2.3 *Computational model*

- Commandline arguments are:

  float: length along x-direction
  float: length along y-direction
  float: length along z-direction (set to zero for 2D)
  integer: number of elements in x-direction
  integer: number of elements in y-direction
  integer: number of elements in z-direction (set to zero for 2D)
  integer: interpolation order (1: linear; 2: quadratic)
  integer: solver type (0: direct; 1: iterative)

- Commandline arguments for tests are:

  2.0 1.0 0.0 2 1 0 1 0
  2.0 1.0 0.0 4 2 0 1 0
  2.0 1.0 0.0 8 4 0 1 0
  2.0 1.0 0.0 2 1 0 2 0
  2.0 1.0 0.0 4 2 0 2 0
  2.0 1.0 0.0 8 4 0 2 0
  2.0 1.0 0.0 2 1 0 1 1
  2.0 1.0 0.0 4 2 0 1 1

2.0 1.0 0.0 8 4 0 1 1

2.0 1.0 0.0 2 1 0 2 1

2.0 1.0 0.0 4 2 0 2 1

2.0 1.0 0.0 8 4 0 2 1

2.0 1.0 1.0 2 1 1 1 0

2.0 1.0 1.0 4 2 2 1 0

2.0 1.0 1.0 8 4 4 1 0

2.0 1.0 1.0 2 1 1 2 0

2.0 1.0 1.0 4 2 2 2 0

2.0 1.0 1.0 8 4 4 2 0

2.0 1.0 1.0 2 1 1 1 1

2.0 1.0 1.0 4 2 2 1 1

2.0 1.0 1.0 8 4 4 1 1

2.0 1.0 1.0 2 1 1 2 1

2.0 1.0 1.0 4 2 2 2 1

2.0 1.0 1.0 8 4 4 2 1

3.2.4 *Result summary*

We use CHeart rev. 6292 to produce numerical reference solutions.

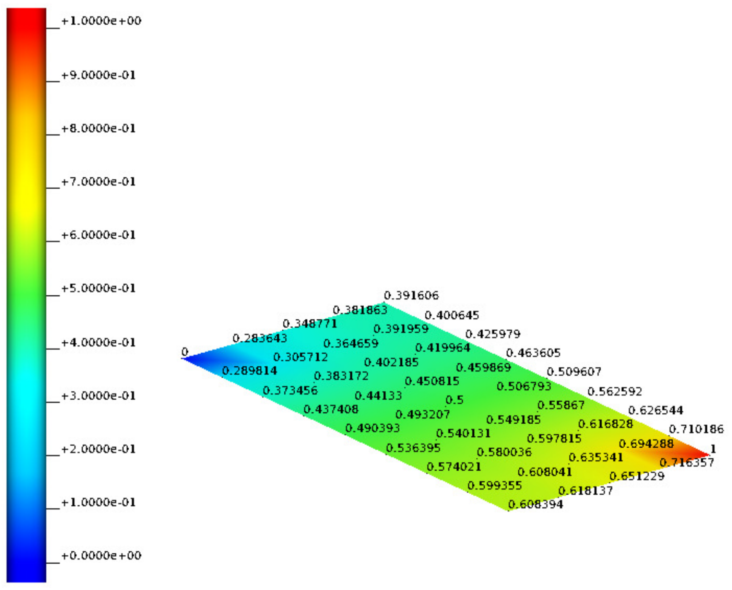


Figure 1: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

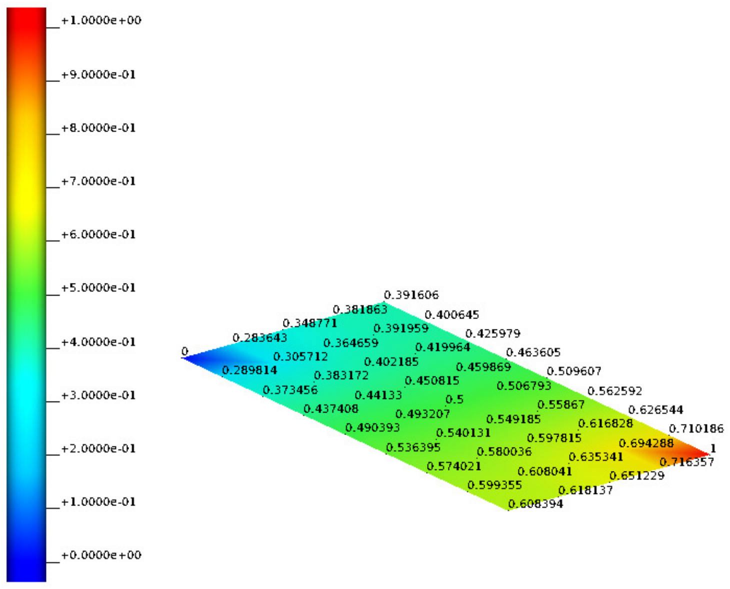


Figure 2: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

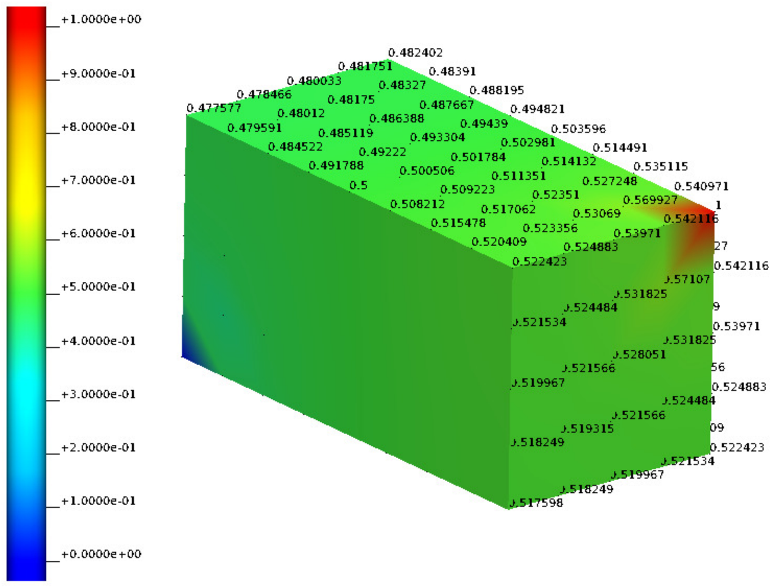


Figure 3: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

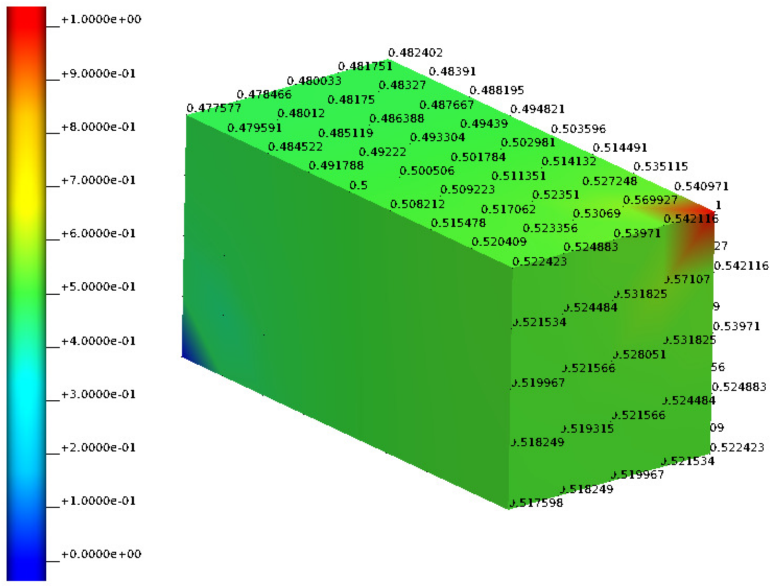


Figure 4: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

3.3 Example-0001-u [VALIDATED]

Example uses user-defined regular meshes in CHeart mesh format and solves a static problem, i.e., applies the boundary conditions in one step.

3.3.1 *Mathematical model - 2D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0, 2] \times [0, 1], \tag{8}$$

with boundary conditions

$$u = 0 \qquad x = y = 0, \tag{9}$$
$$u = 1 \qquad x = 2, y = 1. \tag{10}$$

No material parameters to specify.

3.3.2 *Mathematical model - 3D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{11}$$

with boundary conditions

$$u = 0 \qquad x = y = z = 0, \tag{12}$$
$$u = 1 \qquad x = 2, y = z = 1. \tag{13}$$

No material parameters to specify.

3.3.3 *Computational model*

- Commandline arguments are:

  float: length along x-direction

  float: length along y-direction

  float: length along z-direction (set to zero for 2D)

  integer: number of elements in x-direction

  integer: number of elements in y-direction

  integer: number of elements in z-direction (set to zero for 2D)

  integer: interpolation order (1: linear; 2: quadratic)

  integer: solver type (0: direct; 1: iterative)

- Commandline arguments for tests are:

  2.0 1.0 0.0 2 1 0 1 0

  2.0 1.0 0.0 4 2 0 1 0

  2.0 1.0 0.0 8 4 0 1 0

  2.0 1.0 0.0 2 1 0 2 0

  2.0 1.0 0.0 4 2 0 2 0

  2.0 1.0 0.0 8 4 0 2 0

  2.0 1.0 0.0 2 1 0 1 1

  2.0 1.0 0.0 4 2 0 1 1

2.0 1.0 0.0 8 4 0 1 1

2.0 1.0 0.0 2 1 0 2 1

2.0 1.0 0.0 4 2 0 2 1

2.0 1.0 0.0 8 4 0 2 1

2.0 1.0 1.0 2 1 1 1 0

2.0 1.0 1.0 4 2 2 1 0

2.0 1.0 1.0 8 4 4 1 0

2.0 1.0 1.0 2 1 1 2 0

2.0 1.0 1.0 4 2 2 2 0

2.0 1.0 1.0 8 4 4 2 0

2.0 1.0 1.0 2 1 1 1 1

2.0 1.0 1.0 4 2 2 1 1

2.0 1.0 1.0 8 4 4 1 1

2.0 1.0 1.0 2 1 1 2 1

2.0 1.0 1.0 4 2 2 2 1

2.0 1.0 1.0 8 4 4 2 1

- Note: Binary uses command line arguments to search for the relevant mesh files.

3.3.4 *Result summary*

We use CHeart rev. 6292 to produce numerical reference solutions.

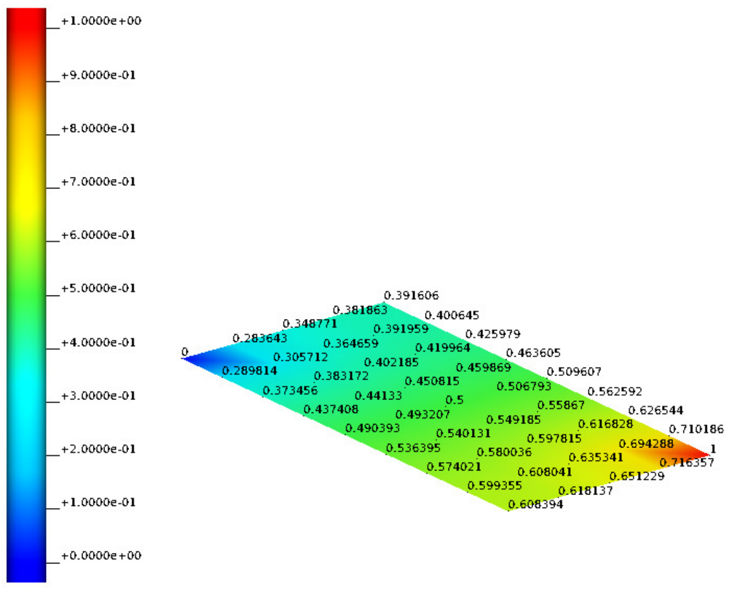


Figure 5: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

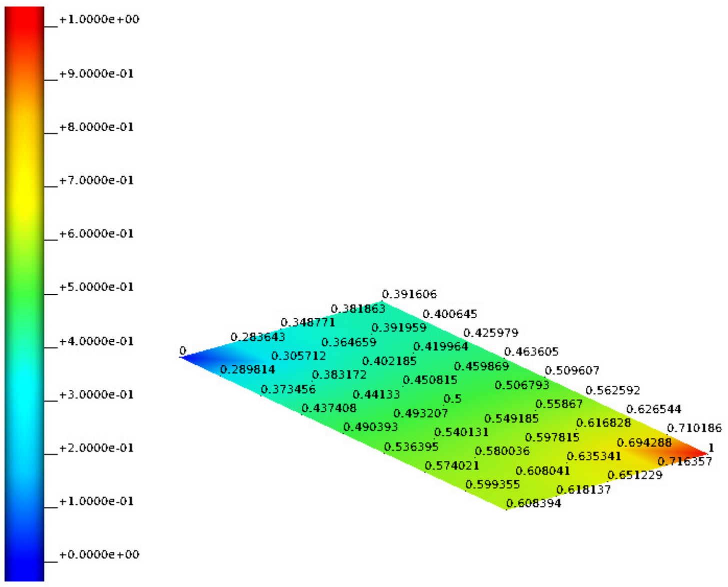


Figure 6: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

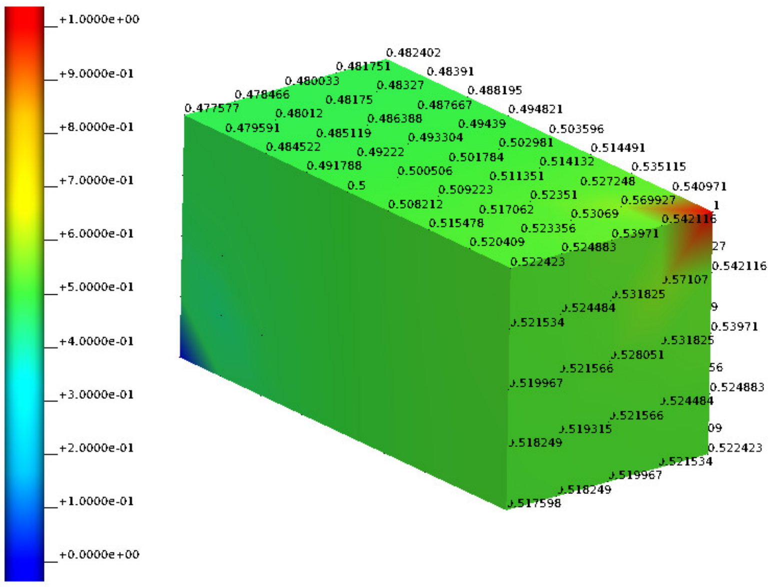


Figure 7: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

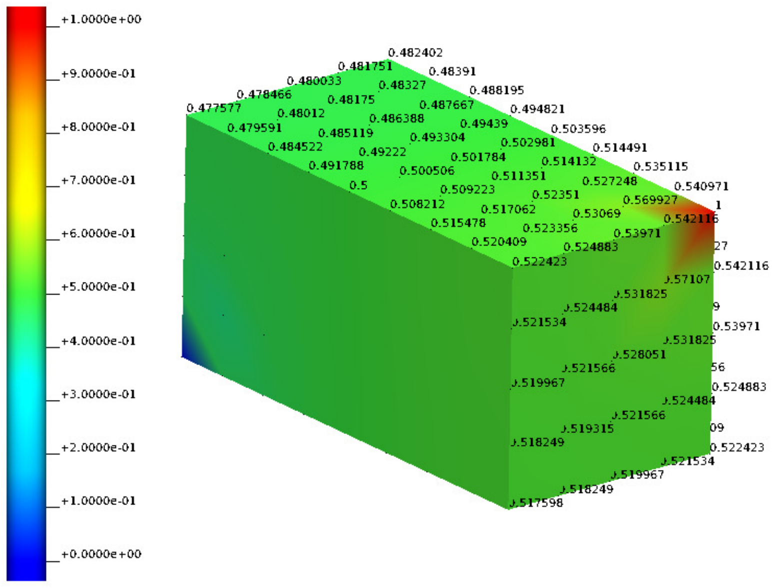


Figure 8: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

3.4 Example-0002 `[VALIDATED]`

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.4.1 *Mathematical model - 2D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0,2] \times [0,1], \tag{14}$$

with boundary conditions

$$u = 15y \qquad x = 0, \tag{15}$$
$$u = 25 - 18y \qquad x = 2. \tag{16}$$

No material parameters to specify.

3.4.2 *Mathematical model - 3D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0,2] \times [0,1] \times [0,1], \tag{17}$$

with boundary conditions

$$u = 15y \qquad x = 0, \tag{18}$$
$$u = 25 - 18y \qquad x = 2. \tag{19}$$

No material parameters to specify.

3.4.3 *Computational model*

- Commandline arguments are:
  float: length along x-direction
  float: length along y-direction
  float: length along z-direction (set to zero for 2D)
  integer: number of elements in x-direction
  integer: number of elements in y-direction
  integer: number of elements in z-direction (set to zero for 2D)
  integer: interpolation order (1: linear; 2: quadratic)
  integer: solver type (0: direct; 1: iterative)
- Commandline arguments for tests are:
  2.0 1.0 0.0 2 1 0 1 0
  2.0 1.0 0.0 4 2 0 1 0
  2.0 1.0 0.0 8 4 0 1 0
  2.0 1.0 0.0 2 1 0 2 0
  2.0 1.0 0.0 4 2 0 2 0
  2.0 1.0 0.0 8 4 0 2 0
  2.0 1.0 0.0 2 1 0 1 1
  2.0 1.0 0.0 4 2 0 1 1

2.0 1.0 0.0 8 4 0 1 1

2.0 1.0 0.0 2 1 0 2 1

2.0 1.0 0.0 4 2 0 2 1

2.0 1.0 0.0 8 4 0 2 1

2.0 1.0 1.0 2 1 1 1 0

2.0 1.0 1.0 4 2 2 1 0

2.0 1.0 1.0 8 4 4 1 0

2.0 1.0 1.0 2 1 1 2 0

2.0 1.0 1.0 4 2 2 2 0

2.0 1.0 1.0 8 4 4 2 0

2.0 1.0 1.0 2 1 1 1 1

2.0 1.0 1.0 4 2 2 1 1

2.0 1.0 1.0 8 4 4 1 1

2.0 1.0 1.0 2 1 1 2 1

2.0 1.0 1.0 4 2 2 2 1

2.0 1.0 1.0 8 4 4 2 1

3.4.4 *Result summary*

We use CHeart rev. 6292 to produce numerical reference solutions.

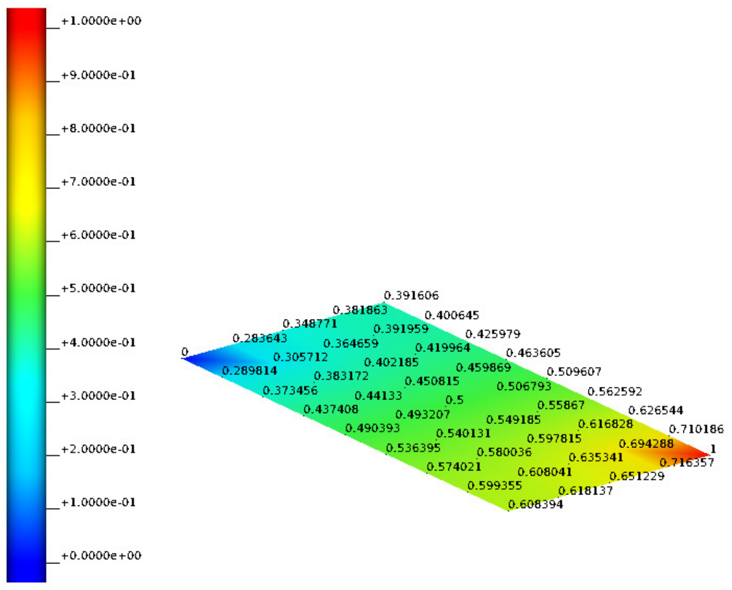


Figure 9: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

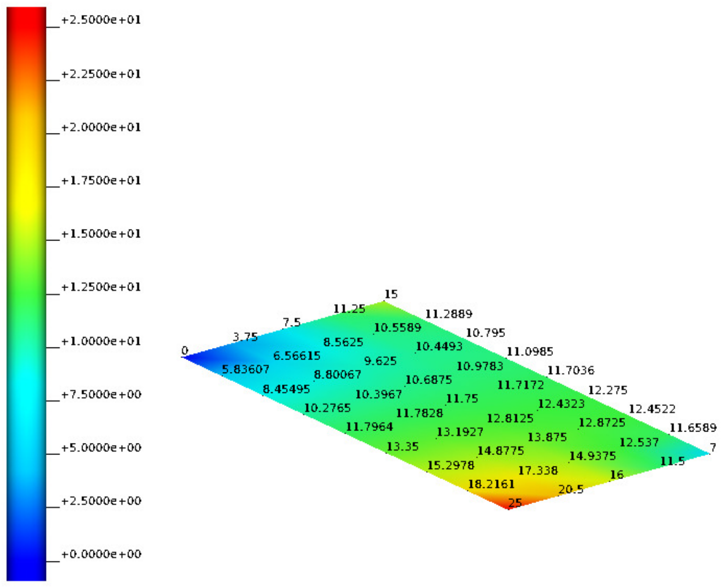


Figure 10: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

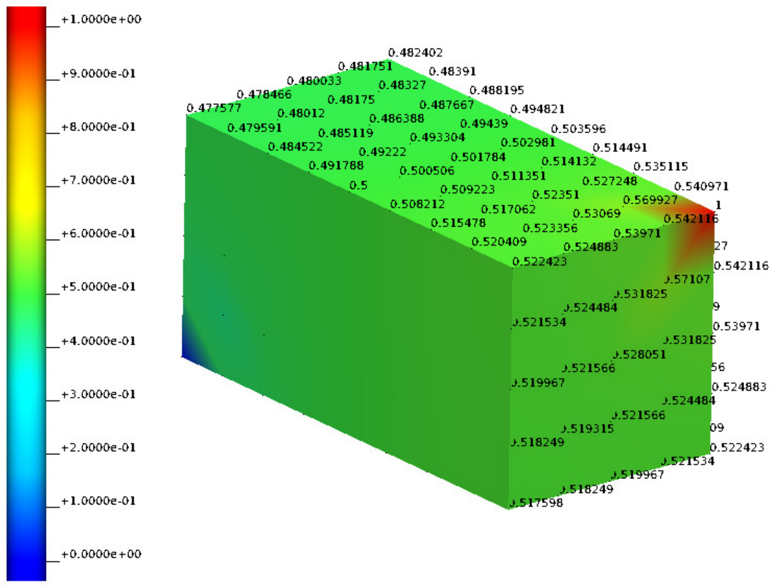


Figure 11: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

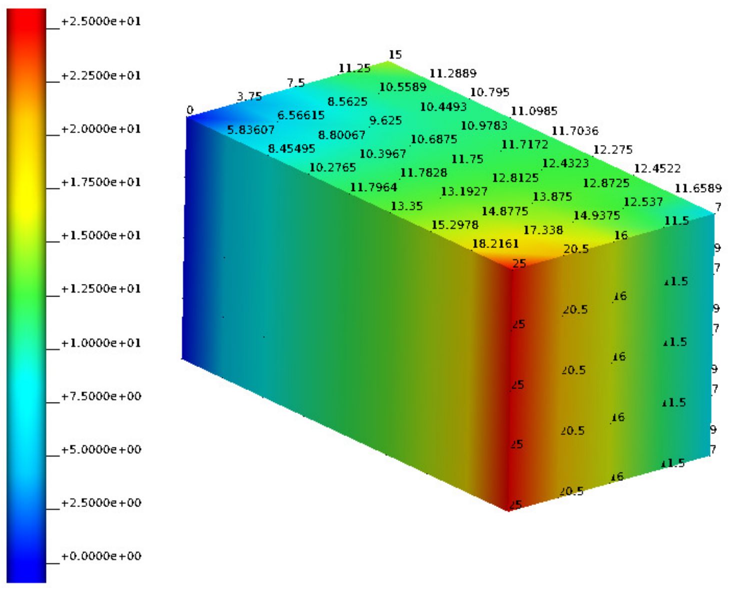


Figure 12: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

3.5 Example-0003 `[COMPILES]`

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.5.1 *Mathematical model - 2D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0,2] \times [0,1], \tag{20}$$

with boundary conditions

$$u = 15y \qquad x = 0, \tag{21}$$
$$\partial_n u = 25 - 18y \qquad x = 2. \tag{22}$$

No material parameters to specify.

3.5.2 *Mathematical model - 3D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0,2] \times [0,1] \times [0,1], \tag{23}$$

with boundary conditions

$$u = 15y \qquad x = 0, \tag{24}$$
$$\partial_n u = 25 - 18y \qquad x = 2. \tag{25}$$

No material parameters to specify.

3.5.3 *Computational model*

- Commandline arguments are:

  float: length along x-direction

  float: length along y-direction

  float: length along z-direction (set to zero for 2D)

  integer: number of elements in x-direction

  integer: number of elements in y-direction

  integer: number of elements in z-direction (set to zero for 2D)

  integer: interpolation order (1: linear; 2: quadratic)

  integer: solver type (0: direct; 1: iterative)

- Commandline arguments for tests are:

  2.0 1.0 0.0 2 1 0 1 0

  2.0 1.0 0.0 4 2 0 1 0

  2.0 1.0 0.0 8 4 0 1 0

  2.0 1.0 0.0 2 1 0 2 0

  2.0 1.0 0.0 4 2 0 2 0

  2.0 1.0 0.0 8 4 0 2 0

  2.0 1.0 0.0 2 1 0 1 1

  2.0 1.0 0.0 4 2 0 1 1

```
2.0 1.0 0.0 8 4 0 1 1
2.0 1.0 0.0 2 1 0 2 1
2.0 1.0 0.0 4 2 0 2 1
2.0 1.0 0.0 8 4 0 2 1
2.0 1.0 1.0 2 1 1 1 0
2.0 1.0 1.0 4 2 2 1 0
2.0 1.0 1.0 8 4 4 1 0
2.0 1.0 1.0 2 1 1 2 0
2.0 1.0 1.0 4 2 2 2 0
2.0 1.0 1.0 8 4 4 2 0
2.0 1.0 1.0 2 1 1 1 1
2.0 1.0 1.0 4 2 2 1 1
2.0 1.0 1.0 8 4 4 1 1
2.0 1.0 1.0 2 1 1 2 1
2.0 1.0 1.0 4 2 2 2 1
2.0 1.0 1.0 8 4 4 2 1
```

3.5.4 *Result summary*

We use CHeart rev. 6292 to produce numerical reference solutions.

Figure 13: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

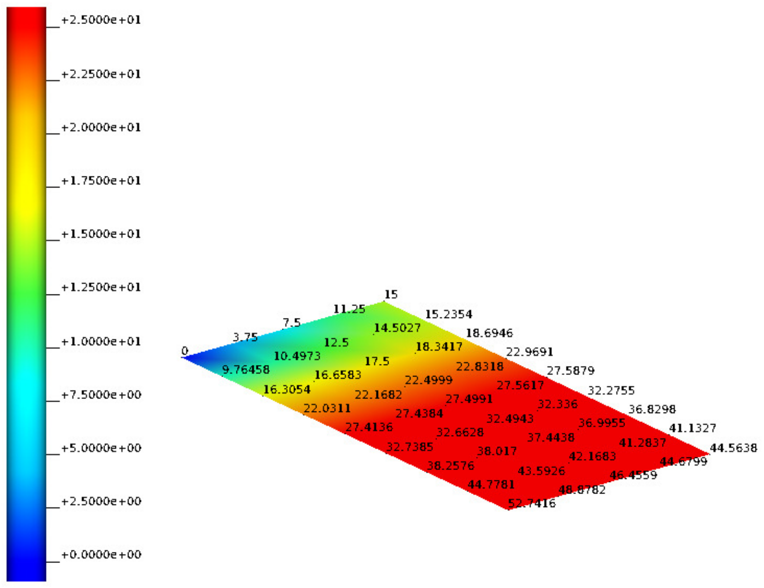


Figure 14: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

Figure 15: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

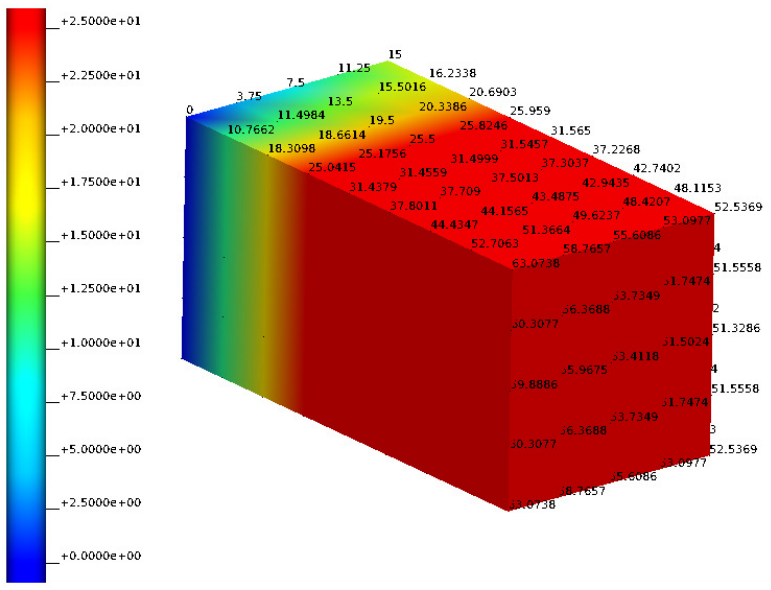


Figure 16: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

3.6 Example-0004 `[VALIDATED]`

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.6.1 *Mathematical model - 2D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0, 2] \times [0, 1], \tag{26}$$

with boundary conditions

$$u = 2.0e^{x} \cdot \cos(y) \qquad \text{on } \partial\Omega. \tag{27}$$

No material parameters to specify.

3.6.2 *Computational model*

- Commandline arguments are:
  integer: number of elements in x-direction
  integer: number of elements in y-direction
  integer: number of elements in z-direction (set to zero for 2D)
  integer: interpolation order (1: linear; 2: quadratic)
  integer: solver type (0: direct; 1: iterative)
- Commandline arguments for tests are:
  4 2 0 1 0
  8 4 0 1 0
  2 1 0 2 0
  4 2 0 2 0
  8 4 0 2 0
  4 2 0 1 1
  8 4 0 1 1
  2 1 0 2 1
  4 2 0 2 1
  8 4 0 2 1
  100 50 0 1 0 (not tested yet..)
  100 50 0 2 0 (not tested yet..)
  100 50 0 1 1 (not tested yet..)
  100 50 0 2 1 (not tested yet..)

3.6.3 *Result summary*

We use CHeart rev. 6292 to produce numerical reference solutions.

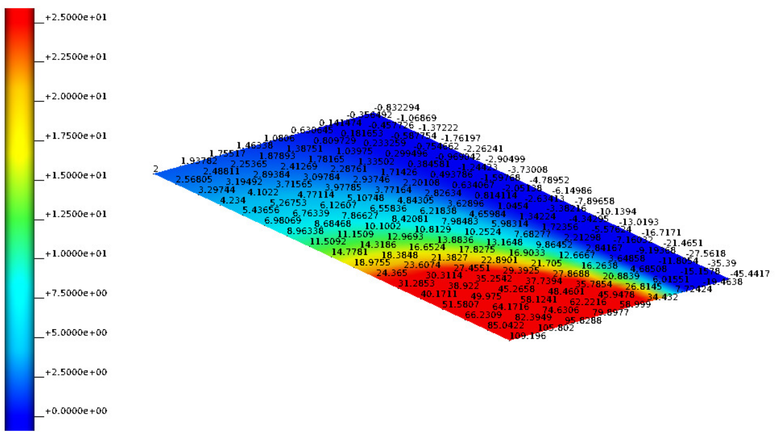


Figure 17: 2D results, iron reference w/ command line arguments [8 4 0 2 0].

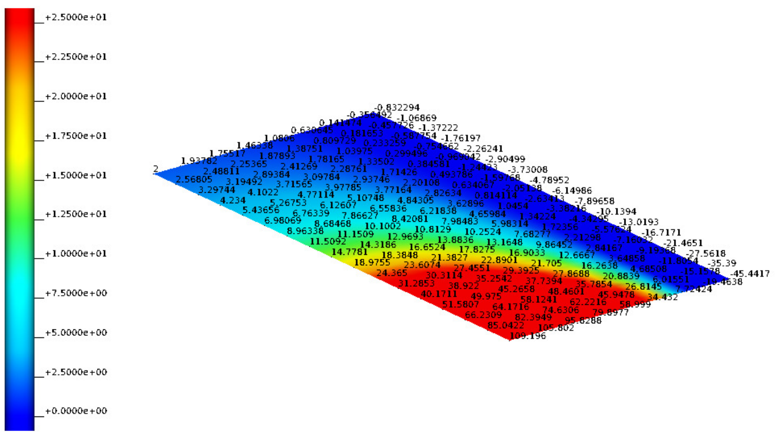


Figure 18: 2D results, current run w/ command line arguments [8 4 0 2 0].

3.7 Example-0005 `[VALIDATED]`

Example uses two user-defined (2d and 3d) unregular meshes and solves a patch test in form of a static problem, i.e., applies the boundary conditions in one step. Here, a Laplace problem with two Dirichlet boundary conditions is solved. The analytical solution for this setting is known and results in a linear distribution of the scalar Laplace parameter u. The numerical solution has to recover this the linear distribution in order to pass the Patch test. 2d and 3d meshes are according to MacNeil and Harder (1985).

3.7.1 *Mathematical model - 2D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0, 0.24] \times [0, 0.12], \tag{28}$$

with boundary conditions

$$u = 0 \qquad x = 0, \tag{29}$$

$$u = 1 \qquad x = 0.24. \tag{30}$$

No material parameters to specify.

3.7.2 *Mathematical model - 3D*

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \Omega = [0, 1] \times [0, 1] \times [0, 1], \tag{31}$$

with boundary conditions

$$u = 0 \qquad x = 0, \tag{32}$$

$$u = 1 \qquad x = 1. \tag{33}$$

No material parameters to specify.

3.7.3 *Computational model*

- Commandline arguments are:

  integer: dimension (2: 2d; 3: 3d)

  integer: interpolation order (1: linear; 2: quadratic)

  integer: solver type (0: direct; 1: iterative)

- Commandline arguments for tests are:

  2 1 0

  2 2 0

  2 1 1

  2 2 1

  3 1 0

  3 2 0

  3 1 1

  3 2 1

3.7.4 *Result summary*

Since the analytical result is known and the numerical results have to recover the linear distribution of u, the comparisons are done with the analytical solution.

```
Passed tests: 8 / 8

No failed tests.
```

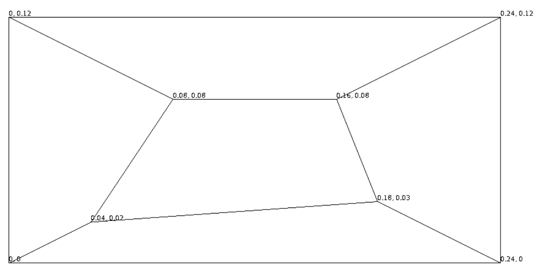


Figure 19: 2D geometry and mesh.

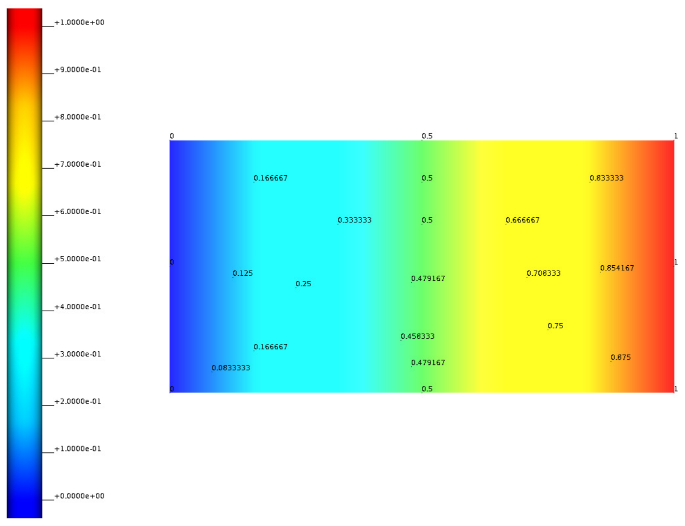


Figure 20: 2D results, iron reference w/ command line arguments [2 2 0].

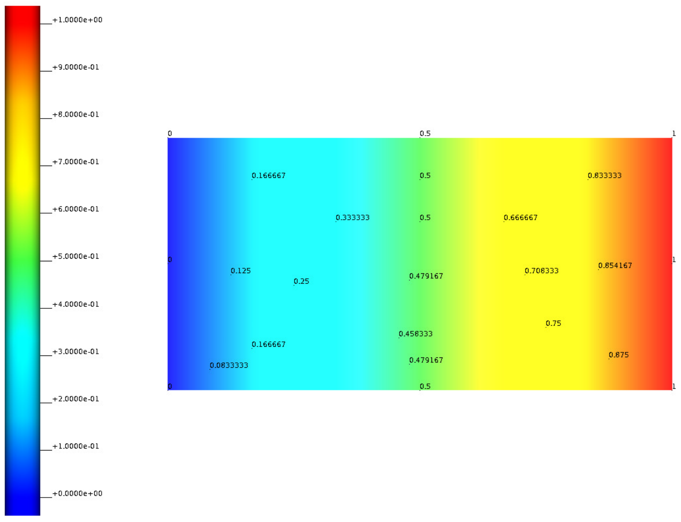


Figure 21: 2D results, current run w/ command line arguments [2 2 0].

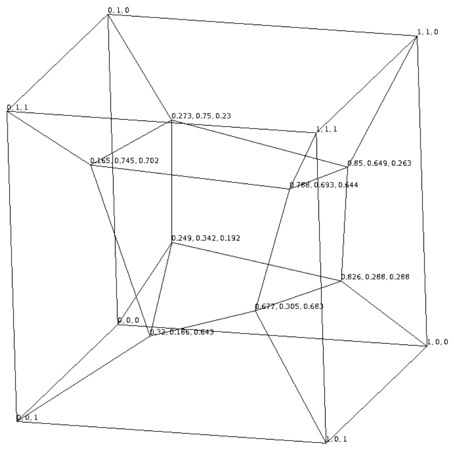


Figure 22: 3D geometry (unit cube) and mesh.

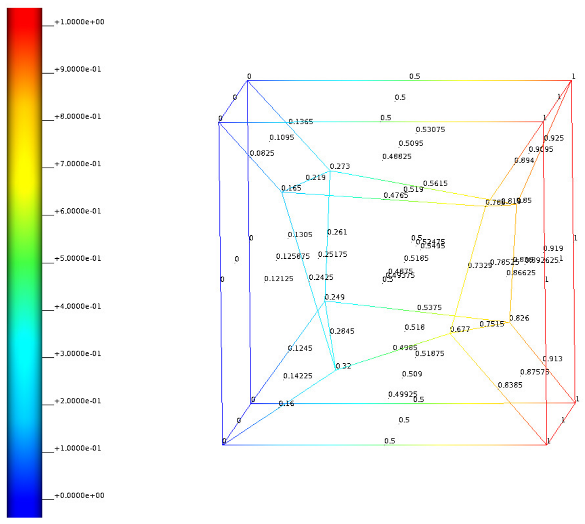


Figure 23: 3D results, iron reference w/ command line arguments [3 2 0].

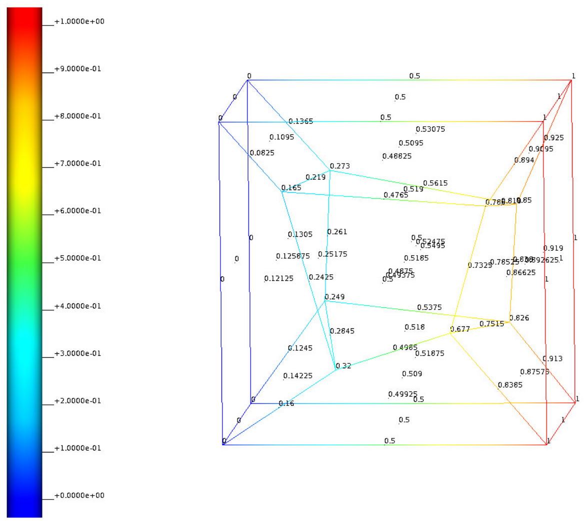


Figure 24: 3D results, current run w/ command line arguments [3 2 0].

3.8 Example-0011 [RUNS]

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.8.1 *Mathematical model - 2D*

We solve the following scalar equation,

$$\nabla \cdot [\boldsymbol{\sigma} \nabla u] = 0 \qquad \Omega = [0, 2] \times [0, 1], \tag{34}$$

with boundary conditions

$$u = 0 \qquad x = y = 0, \tag{35}$$
$$u = 1 \qquad x = 2, y = 1. \tag{36}$$

The conductivity tensor is defined as,

$$\boldsymbol{\sigma}(x, t) = \boldsymbol{\sigma} = \mathbf{I}. \tag{37}$$

3.8.2 *Mathematical model - 3D*

We solve the following scalar equation,

$$\nabla \cdot [\boldsymbol{\sigma} \nabla u] = 0 \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{38}$$

with boundary conditions

$$u = 0 \qquad x = y = z = 0, \tag{39}$$
$$u = 1 \qquad x = 2, y = z = 1. \tag{40}$$

The conductivity tensor is defined as,

$$\boldsymbol{\sigma}(x, t) = \boldsymbol{\sigma} = \mathbf{I}. \tag{41}$$

3.8.3 *Computational model*

- Commandline arguments are:

  float: length along x-direction

  float: length along y-direction

  float: length along z-direction (set to zero for 2D)

  integer: number of elements in x-direction

  integer: number of elements in y-direction

  integer: number of elements in z-direction (set to zero for 2D)

  integer: interpolation order (1: linear; 2: quadratic)

  integer: solver type (0: direct; 1: iterative)

  float: σ_{11}

  float: σ_{22}

  float: σ_{33} (ignored for 2D)

- Commandline arguments for tests are:

  2.0 1.0 0.0 2 1 0 1 0 1 1

  2.0 1.0 0.0 4 2 0 1 0 1 1

```
2.0 1.0 0.0 8 4 0 1 0 1 1
2.0 1.0 0.0 2 1 0 2 0 1 1
2.0 1.0 0.0 4 2 0 2 0 1 1
2.0 1.0 0.0 8 4 0 2 0 1 1
2.0 1.0 0.0 2 1 0 1 1 1 1
2.0 1.0 0.0 4 2 0 1 1 1 1
2.0 1.0 0.0 8 4 0 1 1 1 1
2.0 1.0 0.0 2 1 0 2 1 1 1
2.0 1.0 0.0 4 2 0 2 1 1 1
2.0 1.0 0.0 8 4 0 2 1 1 1
2.0 1.0 1.0 2 1 1 1 0 1 1 1
2.0 1.0 1.0 4 2 2 1 0 1 1 1
2.0 1.0 1.0 8 4 4 1 0 1 1 1
2.0 1.0 1.0 2 1 1 2 0 1 1 1
2.0 1.0 1.0 4 2 2 2 0 1 1 1
2.0 1.0 1.0 8 4 4 2 0 1 1 1
2.0 1.0 1.0 2 1 1 1 1 1 1 1
2.0 1.0 1.0 4 2 2 1 1 1 1 1
2.0 1.0 1.0 8 4 4 1 1 1 1 1
2.0 1.0 1.0 2 1 1 2 1 1 1 1
2.0 1.0 1.0 4 2 2 2 1 1 1 1
2.0 1.0 1.0 8 4 4 2 1 1 1 1
```

3.8.4 *Result summary*

We use CHeart rev. 6292 to produce numerical reference solutions.

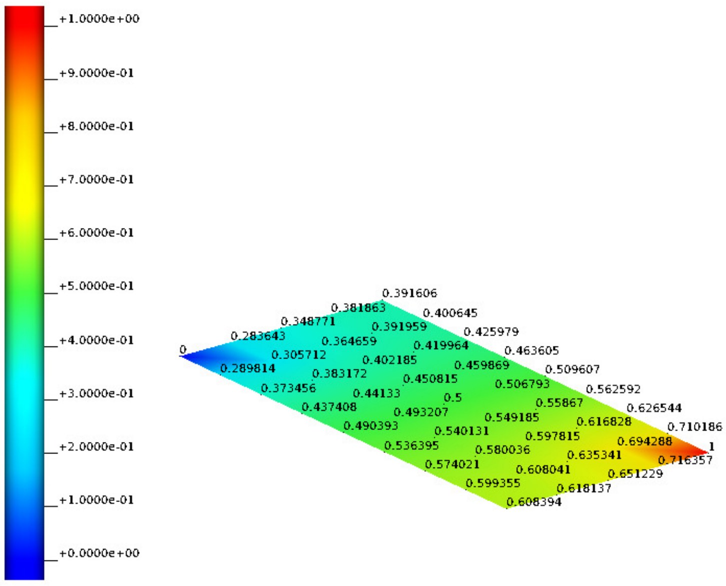


Figure 25: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0 1 1].

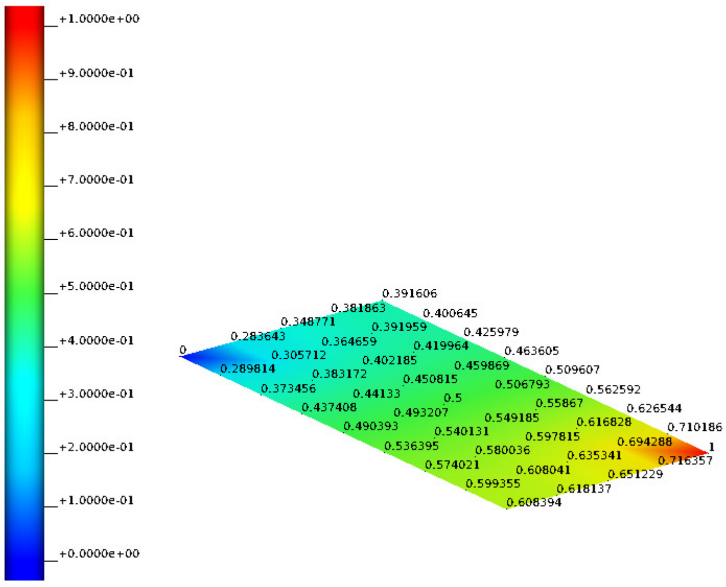


Figure 26: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0 1 1].

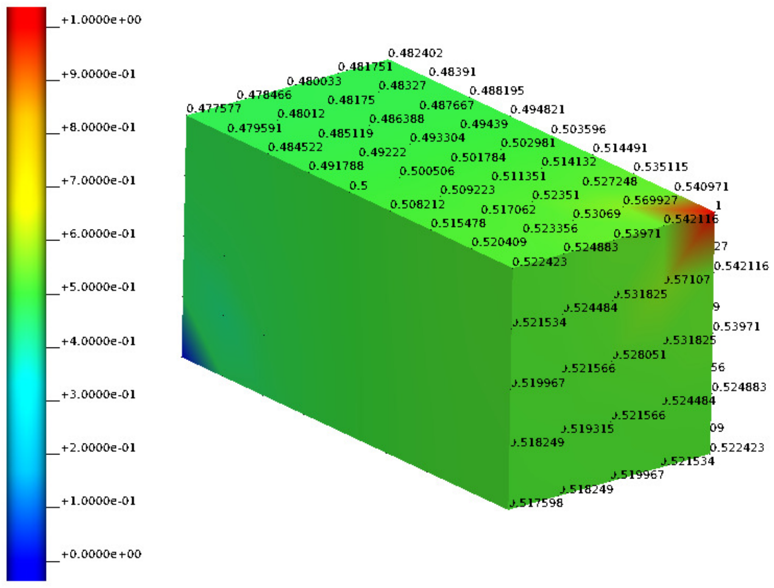


Figure 27: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0 1 1 1].

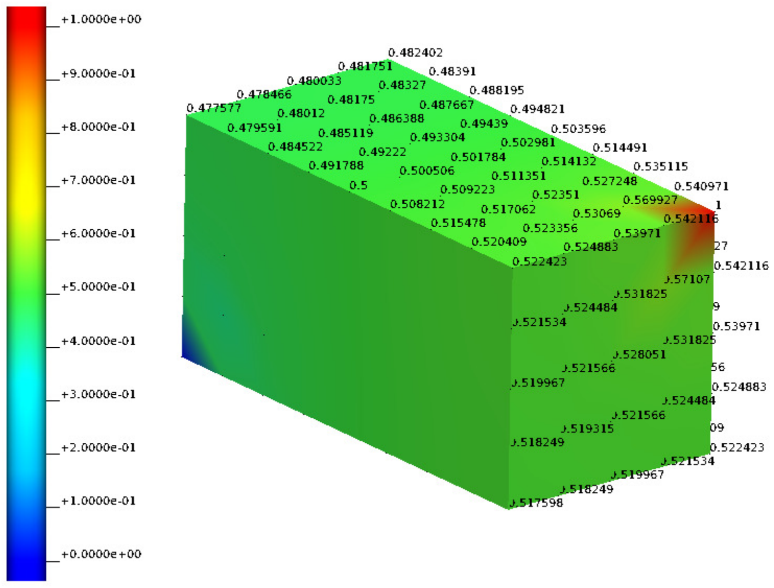


Figure 28: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0 1 1 1].

4 LINEAR ELASTICITY

4.1 Equation in general form

$$\partial_{tt}\mathbf{u} + \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, t) = \mathbf{f}(\mathbf{u}, t) \tag{42}$$

4.2 Example-0101 `[PLAUSIBLE]`

4.2.1 *Mathematical model*

We solve the following equation (both 2D and 3D domains are considered),

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, t) = 0 \qquad \Omega = [0, 160] \times [0, 120] \times [0, 120], t \in [0, 5], \tag{43}$$

with time step size $\Delta_t = 1$ and $\mathbf{u} = [u_x, u_y]$ in 2D $\mathbf{u} = [u_x, u_y, u_z]$ in 3D. The boundary conditions in 2D are given by

$$u_x = u_y = 0 \qquad x = y = 0, \tag{44}$$

$$u_x = 16 \qquad x = 160, \tag{45}$$

and in 3D by

$$u_x = u_y = u_z = 0 \qquad x = y = z = 0, \tag{46}$$

$$u_x = 16 \qquad x = 160. \tag{47}$$

The material parameters are

$$E = 10000\texttt{MPa}, \tag{48}$$

$$\nu = 0.3, \tag{49}$$

$$\rho = 5 \times 10^{-9}\texttt{tonne.mm}^3. \tag{50}$$

4.2.2 *Computational model*

- Commandline arguments are:
  float: length along x-direction
  float: length along y-direction
  float: length along z-direction (set to zero for 2D)
  integer: number of elements in x-direction
  integer: number of elements in y-direction
  integer: number of elements in z-direction (set to zero for 2D)
  integer: interpolation order (1: linear; 2: quadratic)
  integer: solver type (0: direct; 1: iterative)
  float: elastic modulus
  float: Poisson ratio
  float: displacement percentage load
- Command line arguments for tests are:
  160 120 0 8 6 0 1 0 10000 0.3 0.05
  160 120 0 16 12 0 1 0 10000 0.3 0.05
  160 120 0 32 24 0 1 0 10000 0.3 0.05
  160 120 120 8 6 6 1 0 10000 0.3 0.05
  160 120 120 16 12 12 1 0 10000 0.3 0.05
  160 120 120 32 24 24 1 0 10000 0.3 0.05
  160 120 0 8 6 0 2 0 10000 0.3 0.05
  160 120 0 16 12 0 2 0 10000 0.3 0.05
  160 120 0 32 24 0 2 0 10000 0.3 0.05

160 120 120 8 6 6 2 0 10000 0.3 0.05

160 120 120 16 12 12 2 0 10000 0.3 0.05

160 120 120 32 24 24 2 0 10000 0.3 0.05

4.2.3 *Results*

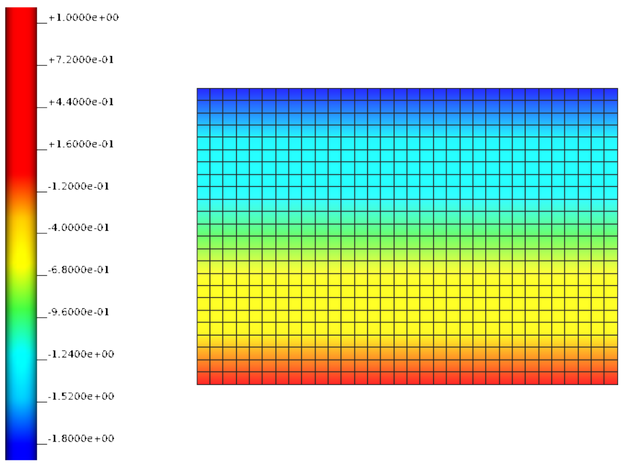


Figure 29: Results, iron 2D fine mesh.

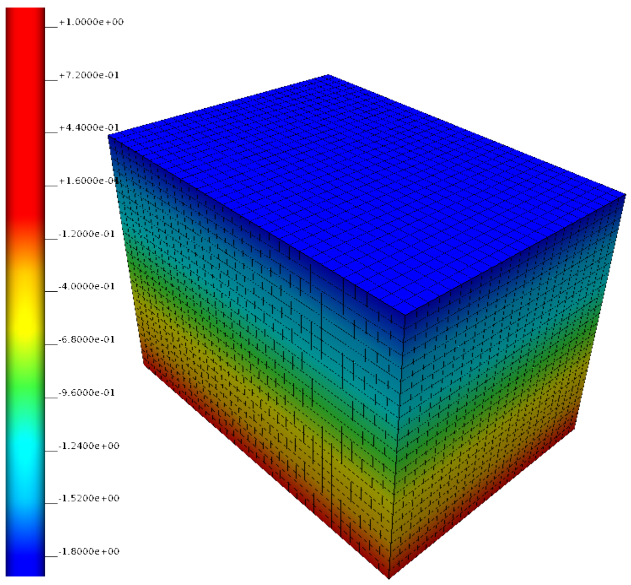


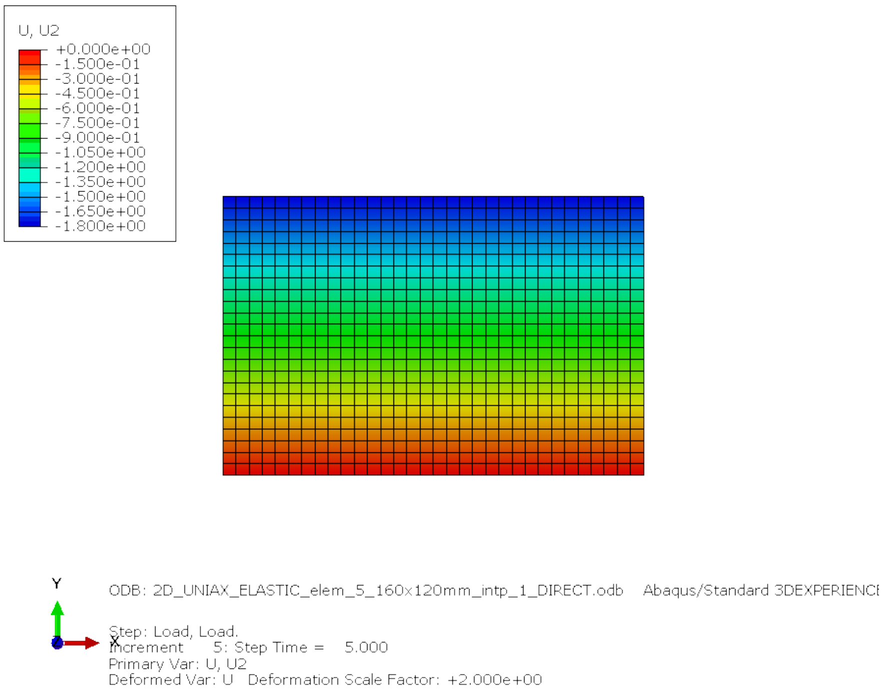
Figure 30: Results, iron 3D fine mesh.

4.2.4 *Validation*

The iron results are compared to those from Abaqus (version 2017). The figures below show selected results from the validation simulations carried out in Abaqus and provide a qualitative validation. A quantitative validation was carried out by comparing the horizontal displacement u_y along the free-edge ($y = 120$ for 2D and $y = z = 120$ for 3D) and computing the L2-norm accodring to

$$L_2\texttt{-norm} = \frac{1}{N} \times \sum_{i=1}^{N} \sqrt{\left(u^i_{y,\texttt{abaqus}} - u^i_{y,\texttt{iron}}\right)^2}, \tag{51}$$

where N is the total number of nodes along the free-edge. The results over the mesh refinements are given in Table 3.



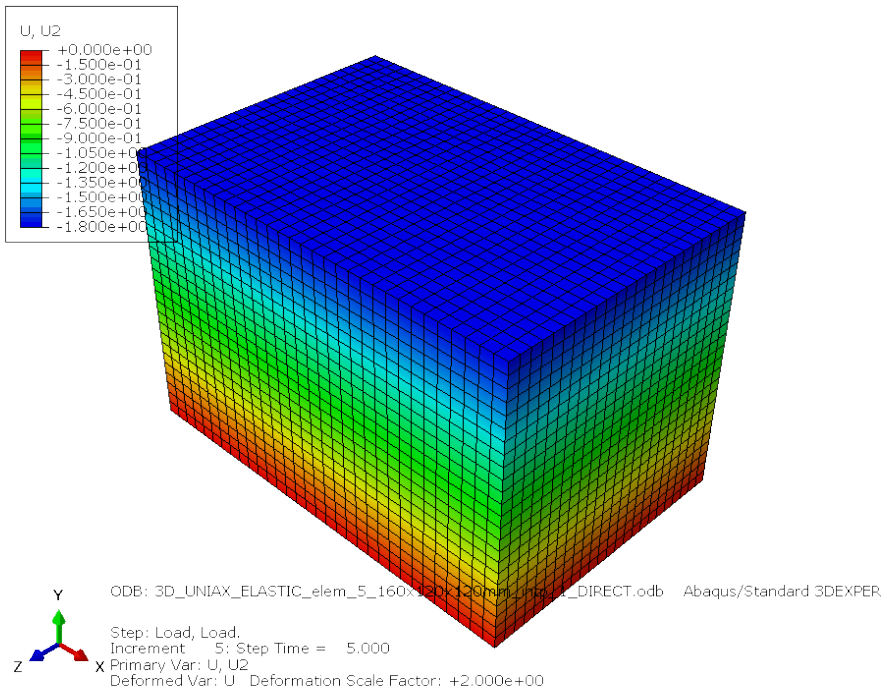
```
ODB: 2D_UNIAX_ELASTIC_elem_5_160x120mm_intp_1_DIRECT.odb    Abaqus/Standard 3DEXPERIENCE

Step: Load, Load.
Increment      5: Step Time =      5.000
Primary Var: U, U2
Deformed Var: U   Deformation Scale Factor: +2.000e+00
```

Figure 31: Results, Abaqus 2D fine mesh.

Dimension	Mesh	$L_2\texttt{-norm}$	Interpolation
2D	Coarse	5.322×10^{-16}	Linear
2D	Medium	1.559×10^{-15}	Linear
2D	Fine	2.900×10^{-15}	Linear
3D	Coarse	3.071×10^{-17}	Linear
3D	Medium	2.125×10^{-17}	Linear
3D	Fine	2.924×10^{-17}	Linear
2D	Coarse	9.728×10^{-16}	Quadratic
2D	Medium	2.039×10^{-15}	Quadratic
2D	Fine	2.159×10^{-15}	Quadratic
3D	Coarse	6.687×10^{-16}	Quadratic
3D	Medium	...	Quadratic
3D	Fine	...	Quadratic

Table 1: Quantiative error between Abaqus 2017 and iron simulations for linear elastic uniaxial extenions



```
ODB: 3D_UNIAX_ELASTIC_elem_5_160x120x120mm_int_1_DIRECT.odb    Abaqus/Standard 3DEXPER

Step: Load, Load.
Increment      5: Step Time =    5.000
Primary Var: U, U2
Deformed Var: U   Deformation Scale Factor: +2.000e+00
```

Figure 32: Results, abaqus 3D fine mesh.

4.3 Example-0102 [PLAUSIBLE]

4.3.1 *Mathematical model*

We solve the following equation (both 2D and 3D domains are considered),

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, t) = \mathbf{0} \qquad \Omega = [0, 160] \times [0, 120] \times [0, 120], t \in [0, 5], \tag{52}$$

with time step size $\Delta_t = 1$ and $\mathbf{u} = [u_x, u_y]$ in 2D $\mathbf{u} = [u_x, u_y, u_z]$ in 3D. The boundary conditions in 2D are given by

$$u_x = u_y = 0 \qquad y = 0, \tag{53}$$
$$u_y = 8 \qquad x = 160, \tag{54}$$

and in 3D by

$$u_x = u_z = 0 \qquad x = 0, \tag{55}$$
$$u_y = 0 \qquad y = 0, \tag{56}$$
$$u_x = 160 \qquad x = 160, \tag{57}$$
$$u_y = 8 \qquad x = 160. \tag{58}$$

The material parameters are

$$E = 10000\texttt{MPa}, \tag{59}$$
$$\nu = 0.3, \tag{60}$$
$$\rho = 5 \times 10^{-9}\texttt{tonne.mm}^3. \tag{61}$$

4.3.2 *Computational model*

- Commandline arguments are:
  float: length along x-direction
  float: length along y-direction
  float: length along z-direction (set to zero for 2D)
  integer: number of elements in x-direction
  integer: number of elements in y-direction
  integer: number of elements in z-direction (set to zero for 2D)
  integer: interpolation order (1: linear; 2: quadratic)
  integer: solver type (0: direct; 1: iterative)
  float: elastic modulus
  float: Poisson ratio
  float: displacement percentage load
- Command line arguments for tests are:
  160 120 0 8 6 0 1 0 10000 0.3 0.05
  160 120 0 16 12 0 1 0 10000 0.3 0.05
  160 120 0 32 24 0 1 0 10000 0.3 0.05
  160 120 120 8 6 6 1 0 10000 0.3 0.05
  160 120 120 16 12 12 1 0 10000 0.3 0.05
  160 120 120 32 24 24 1 0 10000 0.3 0.05
  160 120 0 8 6 0 2 0 10000 0.3 0.05

160 120 0 16 12 0 2 0 10000 0.3 0.05

160 120 0 32 24 0 2 0 10000 0.3 0.05

160 120 120 8 6 6 2 0 10000 0.3 0.05

160 120 120 16 12 12 2 0 10000 0.3 0.05

160 120 120 32 24 24 2 0 10000 0.3 0.05

4.3.3 *Results*

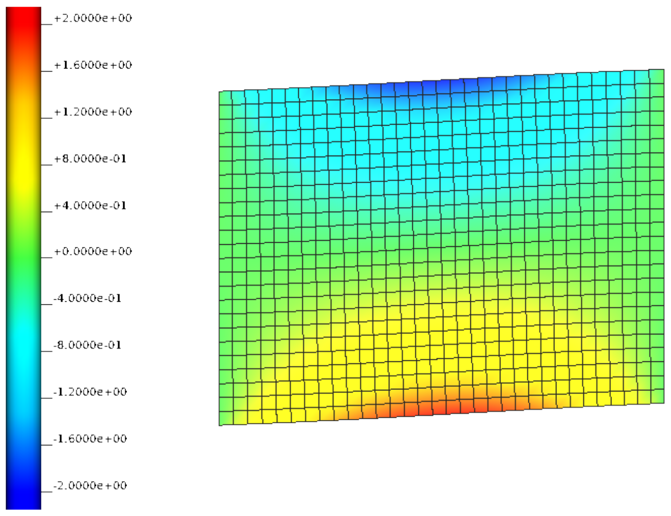


Figure 33: Results, iron 2D fine mesh.

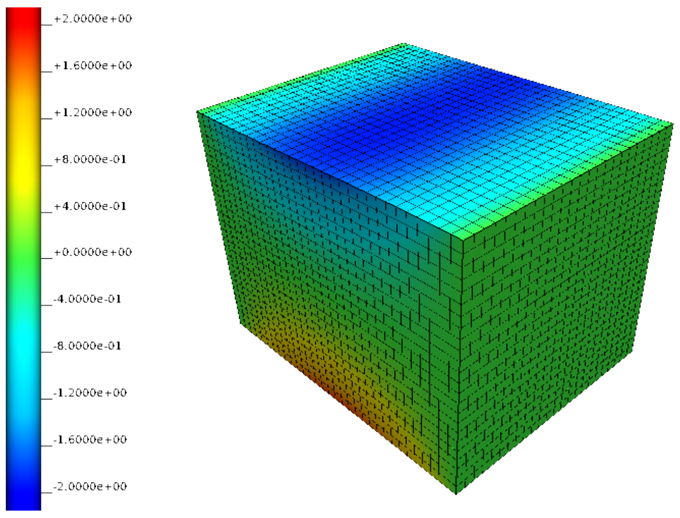


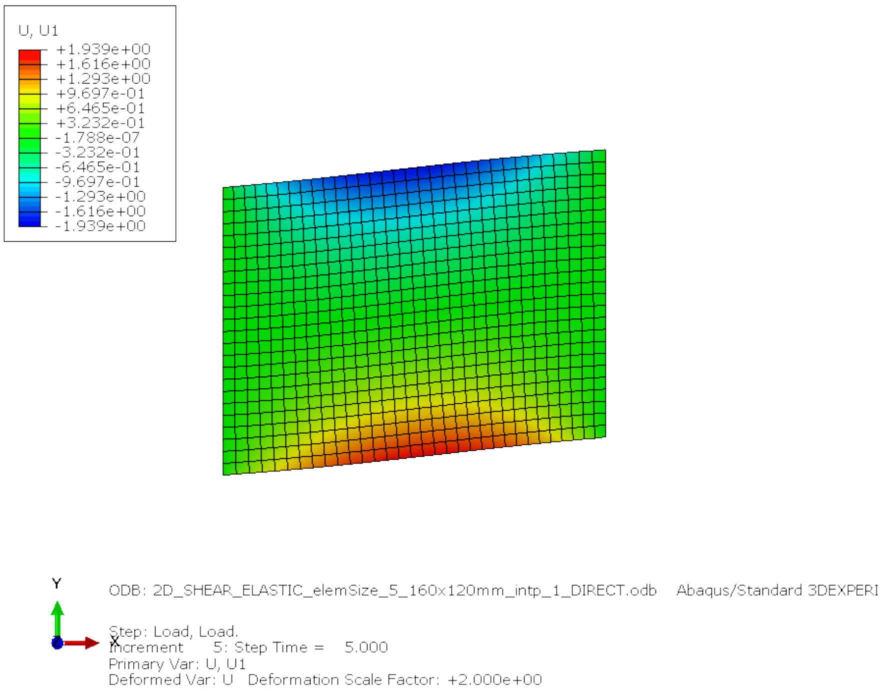
Figure 34: Results, iron 3D fine mesh.

4.3.4 *Validation*

The iron results are compared to those from Abaqus (version 2017). The figures below show selected results from the validation simulations carried out in Abaqus and provide a qualitative validation. A quantitative validation was carried out by comparing the horizontal displacement u_x along the free-edge ($y = 120$ for 2D and $y = z = 120$ for 3D) and computing the L2-norm accodring to

$$\text{L}_2\texttt{-norm} = \frac{1}{N} \times \sum_{i=1}^{N} \sqrt{\left(u^i_{y,\texttt{abaqus}} - u^i_{y,\texttt{iron}}\right)^2}, \tag{62}$$

where N is the total number of nodes along the free-edge. The results over the mesh refinements are given in Table 3.



ODB: 2D_SHEAR_ELASTIC_elemSize_5_160x120mm_intp_1_DIRECT.odb Abaqus/Standard 3DEXPERI

Step: Load, Load.
Increment 5: Step Time = 5.000
Primary Var: U, U1
Deformed Var: U Deformation Scale Factor: +2.000e+00

Figure 35: Results, Abaqus 2D fine mesh.

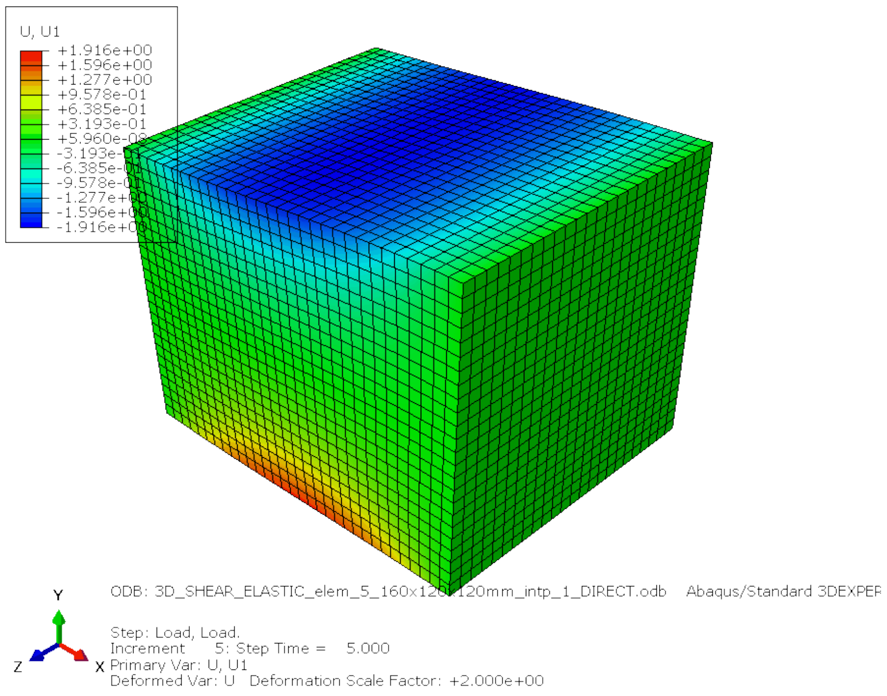


Figure 36: Results, abaqus 3D fine mesh.

Dimension	Mesh	L_2-norm	Interpolation
2D	Coarse	6.696×10^{-3}	Linear
2D	Medium	1.273×10^{-3}	Linear
2D	Fine	2.489×10^{-4}	Linear
3D	Coarse	4.234×10^{-4}	Linear
3D	Medium	4.184×10^{-5}	Linear
3D	Fine	3.781×10^{-6}	Linear
2D	Coarse	3.036×10^{-4}	Quadratic
2D	Medium	6.099×10^{-5}	Quadratic
2D	Fine	1.089×10^{-5}	Quadratic
3D	Coarse	...	Quadratic
3D	Medium	...	Quadratic
3D	Fine	...	Quadratic

Table 2: Quantiative error between Abaqus 2017 and iron simulations for linear elastic shear

4.4 Example-0111 [PLAUSIBLE]

4.4.1 *Mathematical model*

We solve the following equation (both 2D and 3D domains are considered),

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, t) = \mathbf{f}(\mathbf{u}, t) \qquad \Omega = [0, 160] \times [0, 120] \times [0, 120], t \in [0, 5], \tag{63}$$

with time step size $\Delta_t = 1$ and $\mathbf{u} = [u_x, u_y]$ in 2D $\mathbf{u} = [u_x, u_y, u_z]$ in 3D. The boundary conditions in 2D are given by

$$u_x = u_y = 0 \qquad x = y = 0, \tag{64}$$

$$\mathbf{f}(u_x) = 6.0 \times 10^4 \qquad x = 160, \tag{65}$$

and in 3D by

$$u_x = u_y = u_z = 0 \qquad x = y = z = 0, \tag{66}$$

$$\mathbf{f}(u_x) = 7.2 \times 10^6 \qquad x = 160. \tag{67}$$

The material parameters are

$$E = 10000\texttt{MPa}, \tag{68}$$

$$\nu = 0.3, \tag{69}$$

$$\rho = 5 \times 10^{-9}\texttt{tonne.mm}^3. \tag{70}$$

4.4.2 *Computational model*

- Commandline arguments are:
  float: length along x-direction
  float: length along y-direction
  float: length along z-direction (set to zero for 2D)
  integer: number of elements in x-direction
  integer: number of elements in y-direction
  integer: number of elements in z-direction (set to zero for 2D)
  integer: interpolation order (1: linear; 2: quadratic)
  integer: solver type (0: direct; 1: iterative)
  float: elastic modulus
  float: Poisson ratio
  float: XXX
- Command line arguments for tests are:
  160 120 0 8 6 0 1 0 10000 0.3 XXX
  160 120 0 16 12 0 1 0 10000 0.3 XXX
  160 120 0 32 24 0 1 0 10000 0.3 XXX
  160 120 120 8 6 6 1 0 10000 0.3 XXX
  160 120 120 16 12 12 1 0 10000 0.3 XXX
  160 120 120 32 24 24 1 0 10000 0.3 XXX
  160 120 0 8 6 0 2 0 10000 0.3 XXX
  160 120 0 16 12 0 2 0 10000 0.3 XXX

160 120 0 32 24 0 2 0 10000 0.3 XXX
160 120 120 8 6 6 2 0 10000 0.3 XXX
160 120 120 16 12 12 2 0 10000 0.3 XXX
160 120 120 32 24 24 2 0 10000 0.3 XXX

4.4.3 *Results*

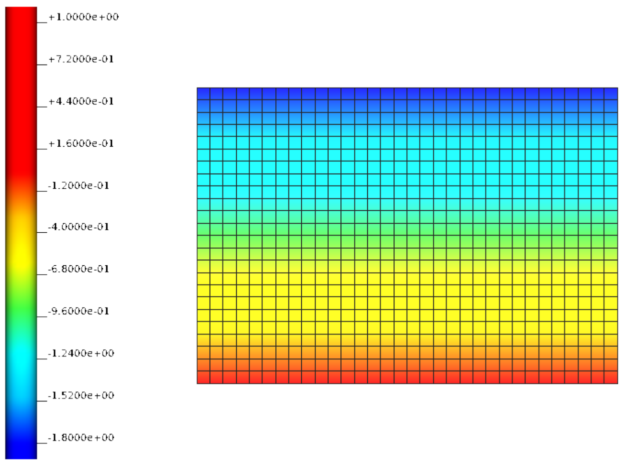


Figure 37: Results, iron 2D fine mesh.

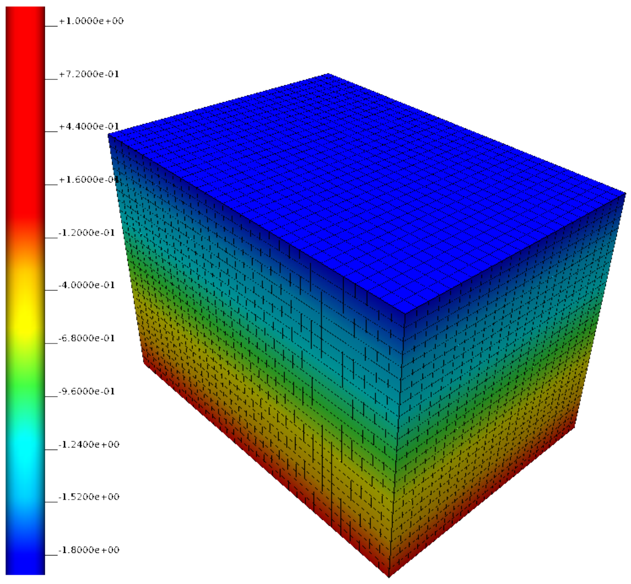


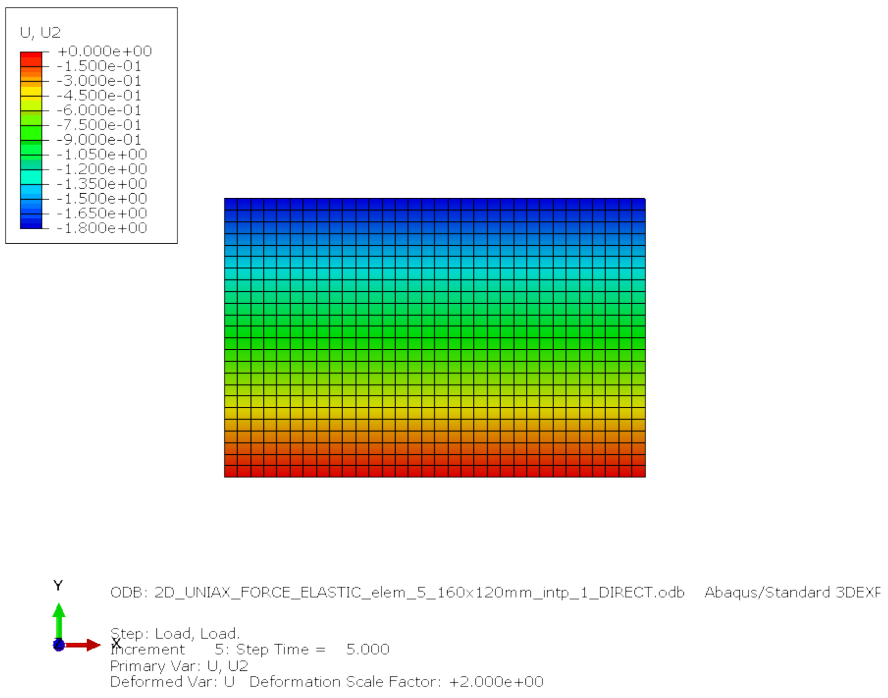
Figure 38: Results, iron 3D fine mesh.

4.4.4 *Validation*

The iron results are compared to those from Abaqus (version 2017). The figures below show selected results from the validation simulations carried out in Abaqus and provide a qualitative validation. A quantitative validation was carried out by comparing the horizontal displacement u_y along the free-edge ($y = 120$ for 2D and $y = z = 120$ for 3D) and computing the L2-norm accodring to

$$L_2\texttt{-norm} = \frac{1}{N} \times \sum_{i=1}^{N} \sqrt{\left(u^i_{y,\texttt{abaqus}} - u^i_{y,\texttt{iron}}\right)^2}, \tag{71}$$

where N is the total number of nodes along the free-edge. The results over the mesh refinements are given in Table 3.



ODB: 2D_UNIAX_FORCE_ELASTIC_elem_5_160x120mm_intp_1_DIRECT.odb   Abaqus/Standard 3DEXF

Step: Load, Load.
Increment   5: Step Time =   5.000
Primary Var: U, U2
Deformed Var: U   Deformation Scale Factor: +2.000e+00

Figure 39: Results, Abaqus 2D fine mesh.

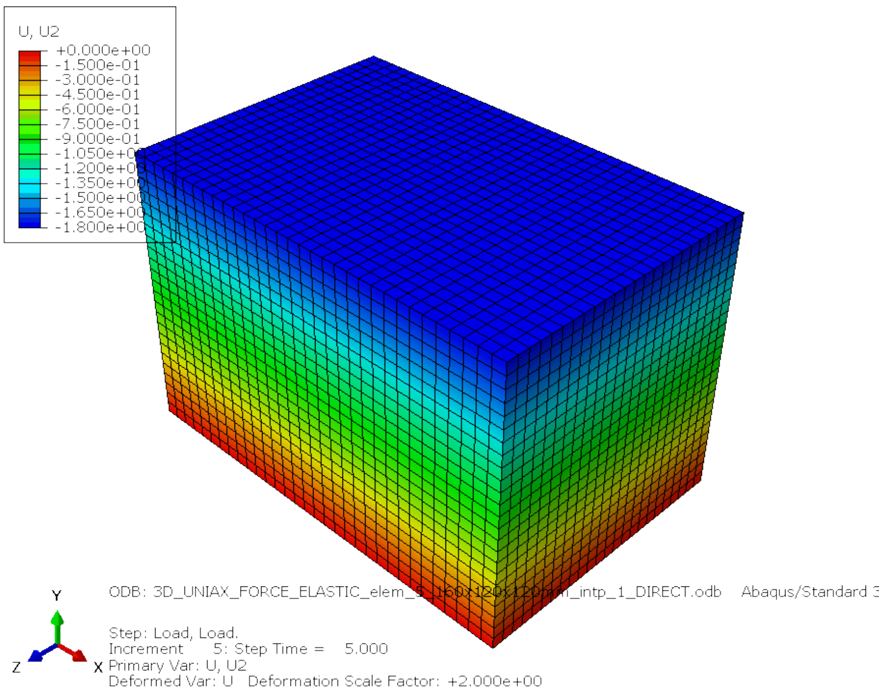


Figure 40: Results, abaqus 3D fine mesh.

Dimension	Mesh	L_2-norm	Interpolation
2D	Coarse	...	Linear
2D	Medium	...	Linear
2D	Fine	...	Linear
3D	Coarse	...	Linear
3D	Medium	...	Linear
3D	Fine	...	Linear
2D	Coarse	...	Quadratic
2D	Medium	...	Quadratic
2D	Fine	...	Quadratic
3D	Coarse	...	Quadratic
3D	Medium	...	Quadratic
3D	Fine	...	Quadratic

Table 3: Quantiative error between Abaqus 2017 and iron simulations for linear elastic uniaxial extenions

4.5 Example-0112 [PLAUSIBLE]

4.5.1 *Mathematical model*

We solve the following equation (both 2D and 3D domains are considered),

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, t) = \mathbf{f}(\mathbf{u}, t) \qquad \Omega = [0, 160] \times [0, 120] \times [0, 120], t \in [0, 5], \tag{72}$$

with time step size $\Delta_t = 1$ and $\mathbf{u} = [u_x, u_y]$ in 2D $\mathbf{u} = [u_x, u_y, u_z]$ in 3D. The boundary conditions in 2D are given by

$$u_x = u_y = 0 \qquad y = 0, \tag{73}$$

$$\mathbf{f}(u_y) = 6.0 \times 10^4 \qquad x = 160, \tag{74}$$

and in 3D by

$$u_x = u_z = 0 \qquad x = 0, \tag{75}$$

$$u_y = 0 \qquad y = 0, \tag{76}$$

$$u_x = 160 \qquad x = 160, \tag{77}$$

$$\mathbf{f}(u_y) = 7.2 \times 10^6 \qquad x = 160. \tag{78}$$

The material parameters are

$$E = 10000\texttt{MPa}, \tag{79}$$

$$\nu = 0.3, \tag{80}$$

$$\rho = 5 \times 10^{-9}\texttt{tonne.mm}^3. \tag{81}$$

4.5.2 *Computational model*

- Commandline arguments are:
  - float: length along x-direction
  - float: length along y-direction
  - float: length along z-direction (set to zero for 2D)
  - integer: number of elements in x-direction
  - integer: number of elements in y-direction
  - integer: number of elements in z-direction (set to zero for 2D)
  - integer: interpolation order (1: linear; 2: quadratic)
  - integer: solver type (0: direct; 1: iterative)
  - float: elastic modulus
  - float: Poisson ratio
  - float: XXX
- Command line arguments for tests are:
  - 160 120 0 8 6 0 1 0 10000 0.3 XXX
  - 160 120 0 16 12 0 1 0 10000 0.3 XXX
  - 160 120 0 32 24 0 1 0 10000 0.3 XXX
  - 160 120 120 8 6 6 1 0 10000 0.3 XXX
  - 160 120 120 16 12 12 1 0 10000 0.3 XXX
  - 160 120 120 32 24 24 1 0 10000 0.3 XXX

160 120 0 8 6 0 2 0 10000 0.3 XXX

160 120 0 16 12 0 2 0 10000 0.3 XXX

160 120 0 32 24 0 2 0 10000 0.3 XXX

160 120 120 8 6 6 2 0 10000 0.3 XXX

160 120 120 16 12 12 2 0 10000 0.3 XXX

160 120 120 32 24 24 2 0 10000 0.3 XXX

4.5.3 *Results*

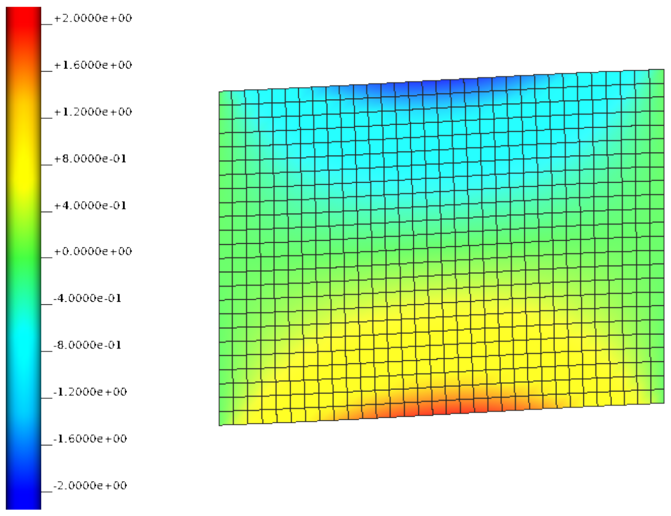


Figure 41: Results, iron 2D fine mesh.

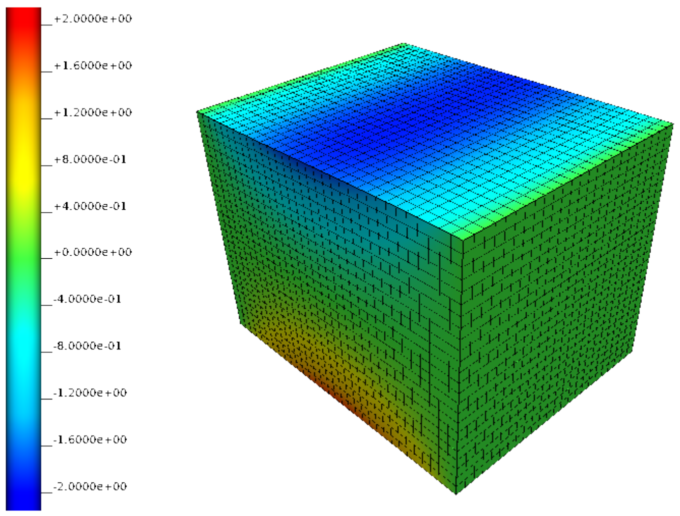


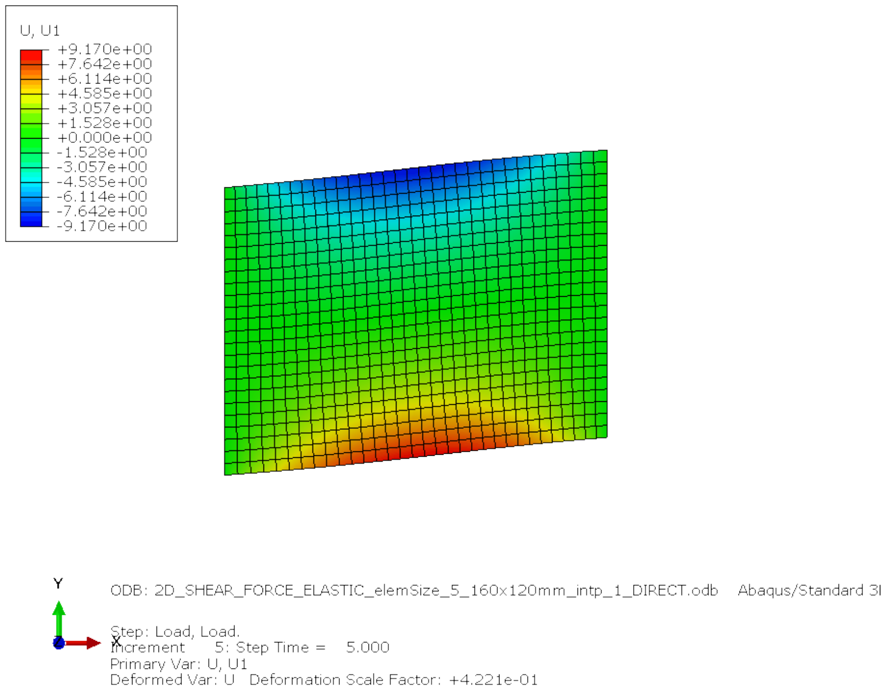
Figure 42: Results, iron 3D fine mesh.

4.5.4 *Validation*

The iron results are compared to those from Abaqus (version 2017). The figures below show selected results from the validation simulations carried out in Abaqus and provide a qualitative validation. A quantitative validation was carried out by comparing the horizontal displacement u_x along the free-edge ($y = 120$ for 2D and $y = z = 120$ for 3D) and computing the L2-norm accodring to

$$\mathtt{L_2\text{-}norm} = \frac{1}{N} \times \sum_{i=1}^{N} \sqrt{\left(u^i_{y,\mathtt{abaqus}} - u^i_{y,\mathtt{iron}}\right)^2}, \tag{82}$$

where N is the total number of nodes along the free-edge. The results over the mesh refinements are given in Table 3.



ODB: 2D_SHEAR_FORCE_ELASTIC_elemSize_5_160x120mm_intp_1_DIRECT.odb Abaqus/Standard 3

Step: Load, Load.
Increment 5: Step Time = 5.000
Primary Var: U, U1
Deformed Var: U Deformation Scale Factor: +4.221e-01

Figure 43: Results, Abaqus 2D fine mesh.

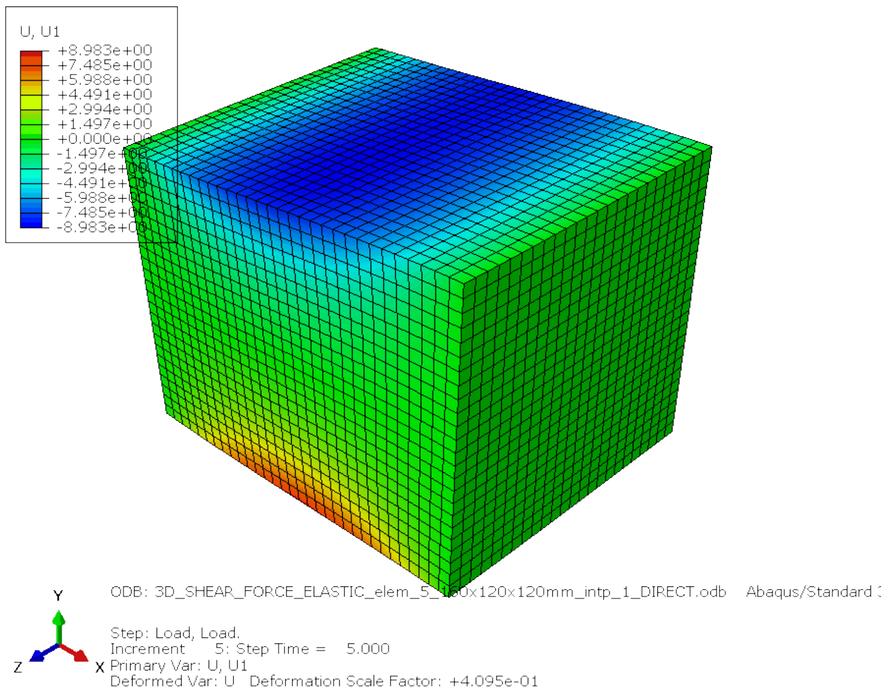


Figure 44: Results, abaqus 3D fine mesh.

Dimension	Mesh	L_2-norm	Interpolation
2D	Coarse	...	Linear
2D	Medium	...	Linear
2D	Fine	...	Linear
3D	Coarse	...	Linear
3D	Medium	...	Linear
3D	Fine	...	Linear
2D	Coarse	...	Quadratic
2D	Medium	...	Quadratic
2D	Fine	...	Quadratic
3D	Coarse	...	Quadratic
3D	Medium	...	Quadratic
3D	Fine	...	Quadratic

Table 4: Quantiative error between Abaqus 2017 and iron simulations for linear elastic shear

5 FINITE ELASTICITY

6 NAVIER-STOKES FLOW

6.1 Equation in general form

$$\partial_t(\rho\boldsymbol{v}) + \nabla\cdot(\rho\boldsymbol{v}\otimes\boldsymbol{v} + p\mathbf{I}) = \rho\mathbf{f} \tag{83}$$

6.2 Example-0302-u `[COMPILES]`

Example uses user-defined simplex meshes in CHeart mesh format with quadratic/linear interpolation for velocity/pressure and solves a dynamic problem.

Setup is the well-known lid-driven cavity problem on the unit square or unit cube in two and three dimensions.

Current issue: does not converge after 30 some time iterations.

6.2.1 *Mathematical model - 2D*

We solve the incompressible Navier-Stokes equation,

$$\partial_t(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v} \otimes \boldsymbol{v}) - \nabla \cdot (\mu \nabla \boldsymbol{v} - p\mathbf{I}) = \rho \mathbf{f} \qquad \Omega = [0,1] \times [0,1], \tag{84}$$
$$\nabla \cdot \boldsymbol{v} = 0, \tag{85}$$

with boundary conditions

$$\boldsymbol{v} = 0 \qquad x = 0, \tag{86}$$
$$\boldsymbol{v} = 0 \qquad x = 1, \tag{87}$$
$$\boldsymbol{v} = 0 \qquad y = 0, \tag{88}$$
$$\boldsymbol{v} = [1,0]^T \qquad y = 1. \tag{89}$$

Viscosity $\mu = 0.0025$, density $\rho = 1$. Thus, Reynolds number $Re = 400$.

6.2.2 *Mathematical model - 3D*

We solve the incompressible Navier-Stokes equation,

$$\partial_t(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v} \otimes \boldsymbol{v}) - \nabla \cdot (\mu \nabla \boldsymbol{v} - p\mathbf{I}) = \rho \mathbf{f} \quad \Omega = [0,1] \times [0,1] \times [0,1], \tag{90}$$
$$\nabla \cdot \boldsymbol{v} = 0, \tag{91}$$

with boundary conditions

$$\boldsymbol{v} = 0 \qquad x = 0, \tag{92}$$
$$\boldsymbol{v} = 0 \qquad x = 1, \tag{93}$$
$$\boldsymbol{v} = 0 \qquad y = 0, \tag{94}$$
$$\boldsymbol{v} = [1,0]^T \qquad y = 1, \tag{95}$$
$$\boldsymbol{v} = 0 \qquad z = 0, \tag{96}$$
$$\boldsymbol{v} = 0 \qquad z = 1. \tag{97}$$

Viscosity $\mu = 0.0025$, density $\rho = 1$. Thus, Reynolds number $Re = 100$.

6.2.3 *Computational model*

- Commandline arguments are:

  integer: number of dimensions (2: 2D, 3: 3D

  integer: mesh refinement level (1, 2, 3, ...)

  float: start time

  float: stop time

  float: time step size

  float: density

  float: viscosity

  integer: solver type (0: direct; 1: iterative)

- Commandline arguments for tests are:

  ```
  2 1 0.0 0.01 0.001 1.0 0.0025 0
  ```

- Note: Binary uses command line arguments to search for the relevant mesh files.

6.2.4 *Result summary*

We use CHeart rev. 6292 to produce numerical reference solutions.

7 MONODOMAIN

8 CELLML MODEL

REFERENCES

[1] Chris Bradley, Andy Bowery, Randall Britten, Vincent Budelmann, Oscar Camara, Richard Christie, Andrew Cookson, Alejandro F Frangi, Thiranja Babarenda Gamage, Thomas Heidlauf, et al. Opencmiss: a multi-physics & multi-scale computational infrastructure for the vph/-physiome project. *Progress in biophysics and molecular biology*, 107(1):32–47, 2011.